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PA Case Number: #16326; Clearance Date: 7/12/16

14. ABSTRACT

Viewgraph/Briefing Charts

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CONSERVATIVE BIN-TO-BIN FRACTIONAL COLLISIONS

Robert Martin

ERC Inc.,
SPACECRAFT PROPULSION BRANCH
AIR FORCE RESEARCH LABORATORY
EDWARDS AIR FORCE BASE, CA USA



30th International Symposium on Rarefied Gas Dynamics Distribution A: Approved for Public Release; Distribution Unlimited: PA #16326





OUTLINE



- BACKGROUND
- **2** Fractional Collisions
- 3 BIN-TO-BIN FRACTIONAL COLLISIONS
- 4 Conclusion



IMPORTANCE OF COLLISION PHYSICS



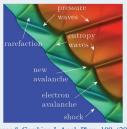
Important Collisions in Spacecraft Propulsion:

- Discharge and Breakdown in FRC
- Collisional Radiative Cooling/Ionization
- Combustion Chemistry

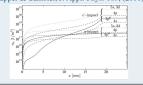
Common Features in Spacecraft Collisions:

- Relevant Densities Spanning Many Orders of Magnitude — 6+
- Transitions from Collisional to Collisionless
- Tiny Early e^- or Radical Populations Critical to Induction Delay
- Many types of Inelastic Collisions with Unknown Effects on Distribution Shapes

Shock Ionization



Kapper & Cambier, J. Appl. Phys. 109, (2011)





IMPORTANCE OF COLLISION PHYSICS



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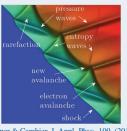
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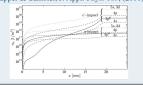
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- Transitions from Collisional to Collisionless
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Need Low Noise & High Dynamic Range Collision Algorithms

Shock Ionization



Kapper & Cambier, J. Appl. Phys. 109, (2011)





STANDARD COLLISION MODELS



Previous Collision Methods:

- Monte Carlo Collisions (MCC)
 - Particles Collide with Background "Fluid"
 - Often Used in Plasma/PIC Simulation
 - Ion-e⁻ Collisions Assume Stationary Ions
 - No Conservation/Detailed Balance
- Direct Simulation Monte Carlo Collisions (DSMC)
 - Most Modern Versions use No-Time Counter (NTC) Method
 - Conservative/Reversible Collision
 - Satisfies Detailed Balance
 - Subset of Possible Collisions Sampled
 - Random Selection vs Z_{ij} for All/Nothing Collision



All Random Flip vs Number of Collisions: $Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle dt$





Continuum to Discrete Representation:

ullet Many Particles $\widetilde{\rightarrow}$ Continuous Distribution





- $\bullet \ \ Many \ Particles \ \widetilde{\rightarrow} \ Continuous \ Distribution$
- Discretized VDF Yields Vlasov
 But Collision Integral Still a Problem





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Variable Weight "All-or-Nothing" Collisions?







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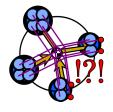
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Variable Weight "All-or-Nothing" Collisions?

Physically Inconsistent!

(Mixing Violates Momentum/Energy Conservation)





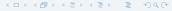


NTC Collisions:

• (Collision Rate Volume):(Cell Volume)

$$Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle_{ij} dt = \frac{w_i w_j}{2V_{cell}^2} \langle \sigma v \rangle_{ij} dt$$

<u>Fractional-NTC Collisions:</u>







NTC Collisions:

- (Collision Rate Volume):(Cell Volume)
- Select Fraction of $\frac{1}{2}N^2$ Possible

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$$P_{max} = w \langle \sigma v \rangle_{ij}^{max} dt / V_{cell}$$

$$N_{select} = \frac{N_p^2}{2} F_n \langle \sigma v \rangle_{ij}^{max} dt / V_{cell}$$

 $P_{ij} = w \langle \sigma v \rangle_{ii} dt / V_{cell}$





NTC Collisions:

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NTC Collisions:

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Fractional-NTC Collisions:

Select f by Cost/Accuracy Tradeoff

$$Z_{ij} = \frac{n_i n_j}{2} \langle \sigma v \rangle_{ij} \, \mathrm{d}t = \frac{w_i w_j}{2 V_{cell}^2} \langle \sigma v \rangle_{ij} \, \mathrm{d}t$$

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- Select f by Cost/Accuracy Tradeoff
- Collision Δw Scaled for Skipped

$$Z_{ij} = rac{n_i n_j}{2} \left< \sigma v \right>_{ij} \mathrm{d}t = rac{w_i w_j}{2 V_{cell}^2} \left< \sigma v \right>_{ij} \mathrm{d}t$$

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 $\Delta w_{ij} = \frac{N_p^2/2}{N_{select}} Z_{ij}$





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Fractional-NTC Collisions:

- Select f by Cost/Accuracy Tradeoff
- Collision Δw Scaled for Skipped
- Add Particles & Original Reduced

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$$\Delta w_{ij} = \frac{N_p^2/2}{N_{select}} Z_{ij}$$
 $w_i = w_i - \Delta w_{ij} \& w_j = w_j - \Delta w_{ij}$
 $w_{(N_p+1)} = \Delta w_{ij} \& w_{(N_p+2)} = \Delta w_{ij}$



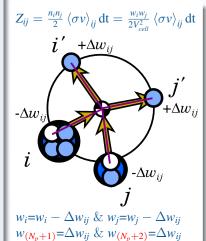


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Fractional-NTC Collisions:

- Select f by Cost/Accuracy Tradeoff
- Collision Δw Scaled for Skipped
- Add Particles & Original Reduced
- +2 Particles/Collision! → Must Merge



$$W(N_p+2)=\Delta W_i$$



Stochastic Weighted Particle Method:

Developed by Rjasanow & Wagner

Attempted Collisions/Cell:

$$\nu = \hat{f}(2\bar{w} - w_{min})N_p(N_p - 1) \langle \sigma v \rangle^{max} dt$$

Select Pair (i,j) if:

Rand
$$< \frac{w_i + w_j - w_{min}}{N_p(N_p - 1)(2\bar{w} - w_{min})}$$

-or-
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Collide If:

Rand
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Perform Standard VHS Collisions

Generate/Modify Particles with:

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Generate/Modify Particles with:

$$\pm \Delta w/f = \pm \min(w_i, w_i)/f$$

Update
$$\langle \sigma v \rangle^{max}$$





Stochastic Weighted Particle Method:

- Developed by Rjasanow & Wagner
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$$(2w_{ma})$$

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- Still Requires Merge $w_i \neq \text{const}$

Attempted Collisions/Cell:

$$\nu = \hat{f}(2\bar{w} - w_{min})N_p(N_p - 1) \langle \sigma v \rangle^{max} dt$$

Select Pair (i,j) if:

$$\begin{aligned} &\text{Rand} < \frac{w_i + w_j - w_{min}}{N_p(N_p - 1)(2\overline{w} - w_{min})} \\ &\quad \text{-or-} \\ &\text{Rand} < \frac{w_i + w_j - w_{min}}{(2w_{max} - w_{min})} \end{aligned}$$

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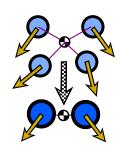


REVIEW OF CONSERVATIVE MERGE



Merge to Pair \rightarrow DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
- Though Energy Conserving, Still Thermalizes VDF



$$\begin{aligned} w_{cell} &= \sum_{i}^{(n+2)} w_i \\ \overline{\vec{v}} &= \frac{1}{w_{cell}} \sum_{i}^{(n+2)} w_i \vec{v}_i \\ \overline{V^2} &= \frac{1}{w_{cell}} \sum_{i}^{(n+2)} w_i \left(\vec{v}_i - \overline{\vec{v}} \right)^2 \\ w_{(a/b)} &= w_m/2 \\ \vec{v}_{(a/b)} &= \overline{\vec{v}} \pm \hat{\mathcal{R}} \sqrt{\overline{V^2}} \\ \text{Similarly: } \vec{x}_{(a/b)} &= \overline{\vec{x}} \pm \hat{\mathcal{R}} \sqrt{\overline{\vec{x}^2}} \end{aligned}$$



REVIEW OF CONSERVATIVE MERGE

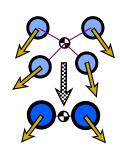


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Selection of Near Neighbors in VDF <u>Limits Thermalization</u>

 $(\approx$ Near Neighbor Pairs in 2:1 Merges that Limit Numerical Cooling)



$$\begin{aligned} w_{cell} &= \sum_{i}^{(n+2)} w_{i} \\ \overline{\vec{v}} &= \frac{1}{w_{cell}} \sum_{i}^{(n+2)} w_{i} \vec{v}_{i} \\ \overline{V^{2}} &= \frac{1}{w_{cell}} \sum_{i}^{(n+2)} w_{i} \left(\vec{v}_{i} - \overline{\vec{v}} \right)^{2} \\ w_{(a/b)} &= w_{m}/2 \\ \vec{v}_{(a/b)} &= \overline{\vec{v}} \pm \hat{\mathcal{R}} \sqrt{\overline{V^{2}}} \\ \text{Similarly: } \vec{x}_{(a/b)} &= \overline{\vec{x}} \pm \hat{\mathcal{R}} \sqrt{\overline{x^{2}}} \end{aligned}$$



REVIEW OF CONSERVATIVE MERGE



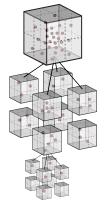
Merge to Pair \rightarrow DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
- Though Energy Conserving, Still Thermalizes VDF

Selection of Near Neighbors in VDF <u>Limits Thermalization</u>

(≈ Near Neighbor Pairs in 2:1 Merges that Limit Numerical Cooling)

Octree Velocity Bins



Efficient Neighbor Selection

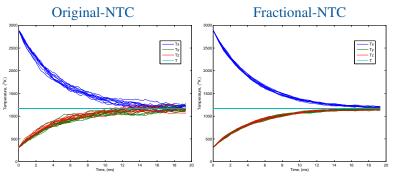




OD-THERMALIZATION



Bi-Maxwellian Thermalization Results



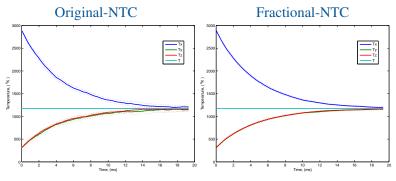
Comparison of 10x Runs from Same Initial Distribution



OD-THERMALIZATION



Bi-Maxwellian Thermalization Results



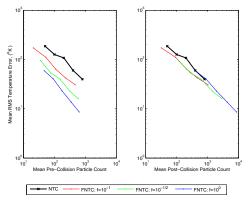
Mean and RMS Fluctuation of Sample Runs Fluctuations Level Tuneable with f Independent of Particles Count



OD-THERMALIZATION



Bi-Maxwellian Thermalization Results



Fluctuations Level Tuneable with f Independent of Particles Count



COLLISIONAL BEAMS IN POTENTIAL WELL

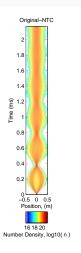


 Initial Bi-Maxwellian Distribution in Potential Well





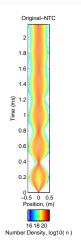
- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization

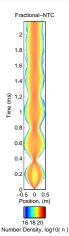






- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior

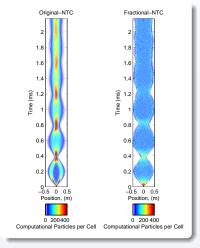








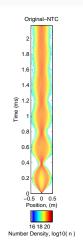
- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior
- Particles/Cell Dramatically Different

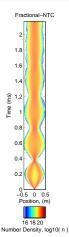






- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior
- Particles/Cell Dramatically Different
- Fringe Extends to Lower Densities with Variable Weights

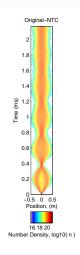


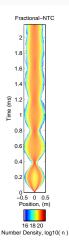






- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior
- Particles/Cell Dramatically Different
- Fringe Extends to Lower Densities with Variable Weights
- Relative 'Error' Unknown without Analytical Solution or High Fidelity Simulation





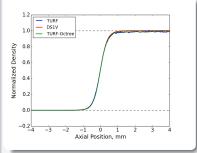


MACH 2 ARGON SHOCK



1D Normal Argon Shock Test

- Simple Verification vs. DS1V
- Initial Conditions: $T_0 = 293 \text{K}, n_0 = 1 \text{E} 22/\text{m}^3, v_0 = 637.4 \text{(m/s)}$
- Initial Jump to Post-Shock at 1cm
- VHS Collisions: T_{ref} =273K, d_{ref} =4.17Å, ω_{VHS} =0.81





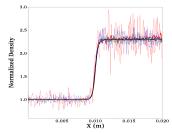
MACH 2 ARGON SHOCK



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- Initial Jump to Post-Shock at 1cm
- VHS Collisions: T_{ref} =273K, d_{ref} =4.17Å, ω_{VHS} =0.81
- Time Average: \bar{n} from $t \in [80, 100) \mu s$

TURF - SWPM+Octree



Target N/Cell Quadrupled per Line

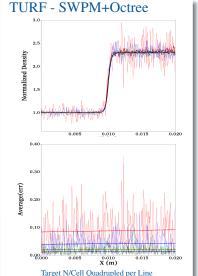


MACH 2 ARGON SHOCK



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- VHS Collisions: T_{ref} =273K, d_{ref} =4.17Å, ω_{VHS} =0.81
- Time Average: \bar{n} from $t \in [80, 100)\mu s$
- Error (Normalized L₁): $err=|n-\bar{n}|/\bar{n}$
- Error Controlled: $err \propto \sqrt{N/cell}$

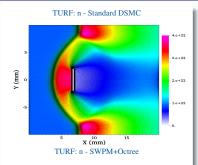






2D Argon Shock Test

- Initial Conditions like M=2 Except: $v_0 = 2550 \text{m/s}$
- Specular: x=5-5.04mm with $y=\pm 2$ mm
- Half Domain Modeled: 80μm × 80μm Cells

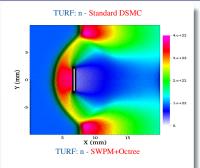






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- Specular: x=5-5.04mm with $y=\pm 2$ mm
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- Time Average: \bar{n} from $t \in [80, 100)\mu s$
- SWPM Similar to Standard DSMC

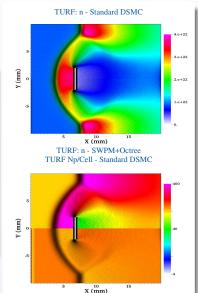






2D Argon Shock Test

- Initial Conditions like M=2 Except: $v_0 = 2550 \text{m/s}$
- Specular: x=5-5.04mm with $y=\pm 2$ mm
- Half Domain Modeled: 80μm × 80μm Cells
- Time Average: \bar{n} from $t \in [80, 100)\mu s$
- SWPM Similar to Standard DSMC
- Despite Different Np/Cell



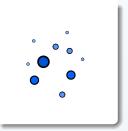
TURF Np/Cell - SWPM+Octree



Issue with Collide then Merge



• Larger $N_{select} \rightarrow$ Better Approx. of Collision Integral

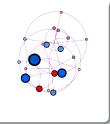




ISSUE WITH COLLIDE THEN MERGE



- Larger $N_{select} \rightarrow$ Better Approx. of Collision Integral
- f-NTC Produces 2x-Particles per $N_{select} = f N_p$
- Particle Memory Requires $\propto N_{max} \rightarrow (1+2f)N_{max}$

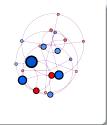




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- For DSMC-like Results, $f \approx O(1)$





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- For DSMC-like Results, $f \approx O(1)$
- Time Accurate or Dense Simulations, $f \approx O(10)+$?

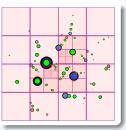




Issue with Collide then Merge



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- Merge Contracts back to $O(N_{max})$ Particles
- Merge Immediately after Collide per Spatial Cell?..
- Sort for Merge still $\propto (1+2f) \log(1+2f)$?

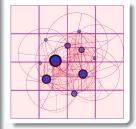




Issue with Collide then Merge



- Larger $N_{select} \rightarrow$ Better Approx. of Collision Integral
- f-NTC Produces 2x-Particles per $N_{select} = f N_p$
- Particle Memory Requires $\propto N_{max} \rightarrow (1+2f)N_{max}$
- For DSMC-like Results, $f \approx O(1)$
- Time Accurate or Dense Simulations, $f \approx O(10)+$?
- Merge Contracts back to $O(N_{max})$ Particles
- Merge Immediately after Collide per Spatial Cell?..
- Sort for Merge still $\propto (1+2f) \log(1+2f)$?
- Combine Collision and Merge in Single Step?







• Fractional Collision as Rate Equation

$$\begin{bmatrix} \vdots \\ \dot{w}_{i} \\ \vdots \\ \dot{w}_{j} \\ \vdots \\ \dot{w}_{i'} \\ \vdots \\ \dot{w}_{j'} \\ \vdots \\ \vdots \end{bmatrix} = \sum_{k=1}^{N_{select}} \begin{bmatrix} \vdots \\ -w_{i} \langle \sigma v \rangle_{ij}^{k} w_{j} \\ \vdots \\ -w_{i} \langle \sigma v \rangle_{ij}^{k} w_{j} \\ \vdots \\ w_{i} \langle \sigma v \rangle_{ij}^{k} w_{j} \\ \vdots \\ w_{i} \langle \sigma v \rangle_{ij}^{k} w_{j} \\ \vdots \\ \vdots \end{bmatrix}$$





- Fractional Collision as Rate Equation
- Bin Moments needed for Particle Pairs

_		
\dot{w}_i		$-\Delta w_{ij}$
\dot{w}_j		$-\Delta w_{ij}$
$\dot{w}_{i'}$		Δw_{ij}
$\dot{w}_{j'}$		Δw_{ij}
_		Δw_{ij}
$(wv)_i$		Δ
$(wv)_i$	N_{select}	$-\Delta w_{ij}v_i$
$(wv)_{i'}$	$=\sum_{i}^{n}$	$-\Delta w_{ij}v_j$
	k=1	$\Delta w_{ij}v_{i'}$
$(wv)_{j'}$		$\Delta w_{ij}v_{j'}$
-		
$(wv^2)_i$		$-\Delta w_{ij}v_i^2$
$(wv^2)_i$		$-\Delta w_{ij}v_j^2$
$(wv^2)_{i'}$		$\Delta w_{ij}v_{i'}^2$
$(wv^2)_{i'}$		$\left[\begin{array}{c} \Delta w_{ij} v_{j'}^2 \end{array}\right]$
\ \ r r r \ / i/		





- Fractional Collision as Rate Equation
- Bin Moments needed for Particle Pairs
- Particle Pairs (i,j) Picked Randomly
- DSMC-like Collision (VHS,VSS,etc.) Random $\chi, \theta \rightarrow (v_{i'}, v_{i'})$

$$\begin{vmatrix} \dot{w}_{i} \\ \dot{w}_{j} \\ \dot{w}_{i'} \\ \dot{w}_{j'} \\ \dot{w$$





- Fractional Collision as Rate Equation
- Bin Moments needed for Particle Pairs
- Particle Pairs (i,j) Picked Randomly
- DSMC-like Collision (VHS,VSS,etc.) Random $\chi, \theta \rightarrow (v_{i'}, v_{i'})$
- Octree to Find i' and j' Bins $8^L \rightarrow \text{Few Levels to Search}$

\dot{w}_i		$-\Delta w_{ij}$
\dot{w}_j		
$\dot{w}_{i'}$		$-\Delta w_{ij}$
$\dot{w}_{j'}$		Δw_{ij}
		Δw_{ij}
		_
$(wv)_i$		$-\Delta w_{ij}v_i$
$(wv)_i$	N_{select}	$-\Delta w_{ij}v_j$
$(wv)_{i'}$	$=$ $\sum_{i=1}^{n}$	
	k=1	$\Delta w_{ij}v_{i'}$
$(wv)_{j'}$		$\Delta w_{ij}v_{j'}$
-		
$(wv^2)_i$		$-\Delta w_{ij}v_i^2$
$(wv^2)_i$		$-\Delta w_{ij}v_i^2$
		$\Delta w_{ij} v_{i'}^2$
$(wv^2)_{i'}$		$\Delta w_{ij}v_{i'}^2$
$(wv^2)_{i'}$		L ┷wŋvj′.





- Fractional Collision as Rate Equation
- Bin Moments needed for Particle Pairs
- Particle Pairs (i,j) Picked Randomly
- DSMC-like Collision (VHS,VSS,etc.) Random $\chi, \theta \rightarrow (v_{i'}, v_{j'})$
- Octree to Find i' and j' Bins $8^L \rightarrow$ Few Levels to Search

Conserve Mass, Momentum, and Energy Memory Constant Independent of N^{select}

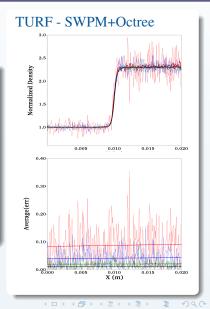
$\begin{bmatrix} \dot{w}_{i} \\ \dot{w}_{j} \\ \dot{w}_{i'} \\ \dot{w}_{j'} \\ - \\ (wv)_{i} \\ (wv)_{j} \\ (wv)_{j'} \\ (wv)_{j'} \\ - \\ (wv^{2})_{i} \\ (wv^{2})_{j} \\ (wv^{2})_{j'} \end{aligned}$	$=\sum_{k=1}^{N_{select}}$	$ \begin{bmatrix} -\Delta w_{ij} \\ -\Delta w_{ij} \\ \Delta w_{ij} \\ \Delta w_{ij}v_{ij} \end{bmatrix} $ $ -\Delta w_{ij}v_{ij} \\ -\Delta w_{ij}v_{ij} \\ \Delta w_{ij}v_{ij} $ $ -\Delta w_{ij}v_{ij}^{2} \\ -\Delta w_{ij}v_{ij}^{2} $ $ \Delta w_{ij}v_{ij}^{2} $
		$\Delta w_{ij} v_{i'}^2 \\ \Delta w_{ij} v_{j'}^2$





1D Normal Argon Shock Test

Mach 2 Case Repeated

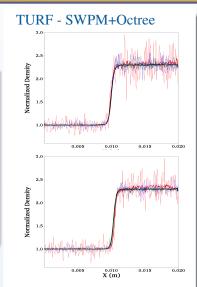






1D Normal Argon Shock Test

- Mach 2 Case Repeated
- Bin-to-Bin Collsions Results Similar



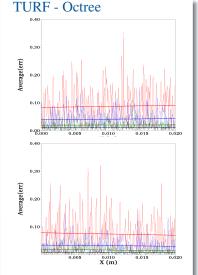
TURF - Bin to Bin





1D Normal Argon Shock Test

- Mach 2 Case Repeated
- Bin-to-Bin Collsions Results Similar
- Target Np/Cell Still Error Control (Target N/Cell Quadrupled per Line)



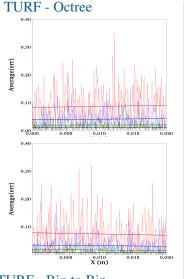
TURF - Bin to Bin





1D Normal Argon Shock Test

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- Target Np/Cell Still Error Control (Target N/Cell Quadrupled per Line)
- Collision Core $\approx 3x$ Slower
- Non-Ideal: Dynamic Range Low

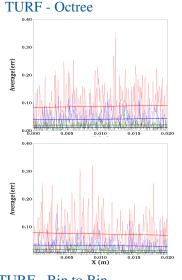






1D Normal Argon Shock Test

- Mach 2 Case Repeated
- Bin-to-Bin Collsions Results Similar
- Target Np/Cell Still Error Control (Target N/Cell Quadrupled per Line)
- Collision Core $\approx 3x$ Slower
- Non-Ideal: Dynamic Range Low
- Proof-of-Concept with Real X-Section
- Expansion/Plume will be Better Case



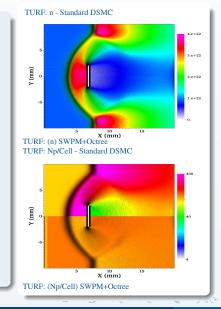
TURF - Bin to Bin





2D Argon Shock Test

Mach 8 Case Also Repeated

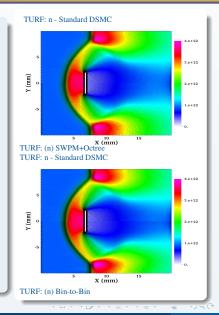






2D Argon Shock Test

- Mach 8 Case Also Repeated
- Bin-to-Bin Collsions Results Similar





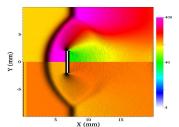
Mach 8 Argon Bow Shock



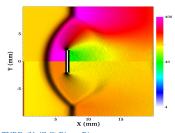
2D Argon Shock Test

- Mach 8 Case Also Repeated
- Bin-to-Bin Collsions Results Similar
- Target Np/Cell Still Error Control

TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) SWPM+Octree TURF: Np/Cell - Standard DSMC





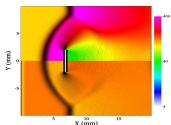


2D Argon Shock Test

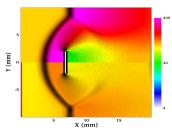
- Mach 8 Case Also Repeated
- Bin-to-Bin Collsions Results Similar
- Target Np/Cell Still Error Control
- B2B Run with f=4x Collisions (Note: SWPM+Octree f=1x)

•	Standard - Collisions	548.9s	1x
	Standard - Total Run	7945.3s	100%
	SWPM+Octree - Collisions	2719.6s	4.95x
	SWPM+Octree - Total Run	9542.4s	120%
	Bin-to-Bin - Collisions	13163.6s	24.0x
	Bin-to-Bin - Total Run	18860.5s	237%

TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) SWPM+Octree TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) Bin-to-Bin





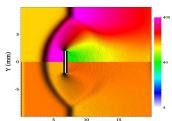
2D Argon Shock Test

- Mach 8 Case Also Repeated
- Bin-to-Bin Collsions Results Similar
- Target *Np/Cell* Still Error Control
- B2B Run with f=4x Collisions (Note: SWPM+Octree f=1x)

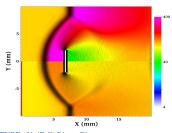
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	Standard - Total Run	7945.3s	100%
•	SWPM+Octree - Collisions	2719.6s	4.95x
•	SWPM+Octree - Total Run	9542.4s	120%
	Bin-to-Bin - Collisions	13163.6s	24.0x
	Bin-to-Bin - Total Run	18860.5s	237%

- Some Cost Compensated by Lower Np
- Too much Fill for Better Wake
- Significant Optimizations Still Needed (i.e. Data Structures, Sort->Sums, v-Bounds, Morton curve)

TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) SWPM+Octree
TURF: Np/Cell - Standard DSMC



TURF: (Np/Cell) Bin-to-Bin



Conclusion



- Standard Collision Incompatible with Variable Weight
- SWPM+Octree Option for Variable Weight Collision
- Bin-To-Bin Potentially Alleviates Memory Constraints
- Initial Verification vs. Standard Shock Cases Positive
- Limited Utility in Standard Shock Cases
- Performance with Strong Expansion/Plume Needed
- SWPM/Bin-to-Bin more Useful for Trace Species?





Thank You

Questions?